An extension of Roe's upwind scheme to algebraic equilibrium real gas models

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Extension du schéma décentré de Roe au cas des gas réels dont l'équation d'état est définie algébriquement

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Résumé

Dans ce rapport, nous montrons comment on peut obtenir une extension du solveur de Roe au cas de gas reéls à l'équilibre chimique à partir d'une généralisation de celui-ci au cas de mélande de gaz parfaits inertes. Nous montrons qu'il n'y a pas unicité de la construction. Nous démontrons la robustesse et efficacité de ce nouveau solveur sur des applications mono et bidimensionnelles

Abstract

In this paper, we show how to derive an extension of Roe's Riemann solver for chemically equilibrium flow from an extension of the same Riemann solver adapted to non reacting mixtures. We explain why there is not uniqueness in the drivation. Some 1D and 2D applications are given to illustrate the robustness and capability of this new solver.

Contents

Nomenclature

- $\mathcal{R}$ is the universal constant of perfect gases
- m_i molar weight of species i
- $R_i = \frac{\mathcal{R}}{m_i}$
- c_{v_i} and c_{p_i} are the specific heats of species i.
- $\gamma_i = \frac{c_{pi}}{c_{v_i}}$
- $\kappa_i = \gamma_i - 1$
- T is the temperature of the flow
- ρ_i is the density of species i
- ρ is the total density, $\rho = \sum_{i=1}^{ns} \rho_i$
- $Y_i = \frac{\rho_i}{\rho}$ is the mass fraction of species i
- h_i^0 is the enthalpy of formation of species i
- θ_i is a typical value of the vibrational temperature of the molecules of species i
- p is the pressure
- u is the velocity, $m = \rho u$ is the momentum
- e is the total energy per unit volume
- ϵ is the specific energy per unit volume
- e_{vib}^i specific vibrational energy of species i
- $H = \frac{e+p}{\rho}$ is the specific enthalpy
- $\Delta f = f_R - f_L$

Chapter 1

Introduction

The development of trans-atmospheric vehicle projects (HERMES, NASP, SANGER, etc) has considerably revived research in hypersonics. In particular, many groups are currently working on the development of numerical schemes for solving the P.D.E. systems which describe the flows around such vehicles.

A good description of the main features of these flows (except boundary layer) can be achieved by mean of the Euler system of equations. The success of upwind schemes for solving them in transsonic and supersonic applications give the legitimate desire of extending them to hypersonic purposes. New phenomena occur : chemical reactions, vibrational relaxation or ionisation may be not negligible. At sufficiently low altitudes, the assumption of thermal and chemical equilibrium can be considered to be valid. Under this assumption, the thermodynamical state of air only depends on two independent variables, for example density and internal energy. This paper is devoted to the derivation of numerical algorithms adapted their simulation.

One of the fundamental ingredients of an upwind scheme is the approximate Riemann solver which is used in it. Among all solvers, one of the most popular is Roe's [12].

This solver has already been extended to mixture of non reacting gas with more or less complex equation of state (see [13,15], [3,1,7,18])). The solutions given in [1] or [3] are very similar. They only differ by the expression of the averaged derivatives of the pressure towards the conservative variables. The solutions in [1] and [2] gives the same expression of the averaged partial derivatives but lead to different expressions of the averaged speed of sound. The technique developed in [13] has been extensively used for 3D applications [8].

Various authors have given solutions to extend Roe's approximate Riemann solver to chemical equilibrium flows (see Glaister [11], Shuen and al. [10], Vinokur et al. [9,16], Grosmann et al. [4] for example)

For all these authors, the thermodynamics properties of air is described either by analytical expressions [11] or by means of curve fits [11,10,18,4]. They never use, in their derivations, any information given by the composition of the gas itself. The smoothness

of the curve fits they use may be very important.

In [4], it is assumed that the thermodynamical properties of air does not change too much between two states. This assumption may be completely wrong in some extreme cases.

Here, we propose a completely different approach which is based on two main features : first, we assume to know which species compose the mixture and second, the chemistry model is an algebraic one. This enable us to have a complete and smooth description of the flow. Here, we will use Park's [5] model but the methodology can be applied to any other algebraic model.

To derive our version of Roe's Riemann solver, we start from its expression in the case of a mixture of perfect non reacting gases [14]. Then we show how to build a family of Riemann solvers and we exhibit parameters which do not allow to have uniqueness of the derivation.

Like the authors we have mentioned above, we cannot prove that our version of Roe's Jacobian matrix has real eigenvalues. We believe that for a convex equation of state this should be true because the description of the thermodynamics is very smooth and because we can prove that the eigenvalues of the "frozen" Roe's Jacobian matrix are real (see appendix).

The robustness and the efficiency of this new solver is shown on 1D and 2D test cases.

Chapter 2

Equation of state, physical model and Jacobian matrix

2.1 Equation of state

We consider a mixture of ns perfect gases. The internal energy of a given species is :

$$\epsilon_i = \rho_i c_{v_i} T + \rho_i {h_i}^0 + \rho_i e^i_{vib}$$

where T is the translational temperature, ${h_i}^0$ is the enthalpy of formation of this particular species at a reference temperature and e^i_{vib} is the specific vibrational of species i (this term disappear for the monoatomic species).

The internal energy ϵ is the sum of the each internal energy :

$$\epsilon = \sum_{i=1}^{ns} \rho_i c_{v_i} T + \sum_{i=1}^{ns} \rho_i {h_i}^0 + \sum_{i=1}^{nv} \rho_i {e_{vib}}^i \tag{2.1}$$

In equation (2.1), nv is the number of diatomic species which are assumed to be the nv first ones.

For practical applications, we consider the following approximation of the specific vibrational energy [17] :

$${e_{vib}}^i = \frac{R_i \theta_i}{exp(\frac{\theta_i}{T}) - 1}$$

The pressure is given by Dalton's law :

$$p = \sum_{i=1}^{ns} \rho_i c_{v_i} \kappa_i T = \rho c_v \kappa T, \tag{2.2}$$

where $c_v = \sum_{i=1}^{ns} Y_i c_{v_i}$ and $\kappa = \frac{\sum_{i=1}^{ns} Y_i c_{v_i} \kappa_i}{\sum_{i=1}^{ns} Y_i c_{v_i}}$.

2.2 Chemical model

In the following, we will consider air as a mixture of five species though all what we say can be easily generalized to much more complex models taking into account, for example, ionisation. Here, we consider five species : O, N, NO, O_2 and N_2.

Moreover, we assume the mixture to be in chemical and thermal equilibrium. Here, we assume three chemical reactions :

$$\begin{aligned} O_2 &\rightleftharpoons 2\,O \\ N_2 &\rightleftharpoons 2\,N \\ NO &\rightleftharpoons N + O \end{aligned}$$

The distribution of mass between each component is given by :

$$\begin{aligned} \frac{[O]^2}{[O_2]} &= K_1(T) \\ \frac{[N]^2}{[N_2]} &= K_2(T) \\ \frac{[O]\,[N]}{[NO]} &= K_3(T) \end{aligned} \tag{2.3}$$

For practical applications, we will use the equilibrium constants given by Park [5] ; but any other algebraic model could have been used.

We have to add another relation which expresses that the global composition of the mixture remains constant :

$$\alpha\,([O] + [NO] + 2[O_2]) = \beta\,([N] + [NO] + 2[N_2]) \tag{2.4}$$

For standard air, the constants α and β are respectively $1/21$ and $1/79$.

2.3 Euler equations

Since we assume thermal and chemical equilibrium, the thermodynamical state of the system depends on two independent variables, for example density ρ and internal energy ϵ. It could have also been density and temperature.

Consequently, the independent variables which describe the system are density, momentum ρu and total energy $e = \epsilon + \frac{1}{2}\rho u^2$, the evolution of which is given by the classical Euler equation where there is a non linear dependence of the pressure, density and total energy :

$$\frac{\partial W}{\partial t} + \frac{\partial F}{\partial x} = 0$$

with

$$W = \begin{pmatrix} \rho \\ \rho u \\ e \end{pmatrix} \qquad F(W) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(e+p) \end{pmatrix} \qquad p = p(\rho, e)$$

Jacobian matrix We immediately get

$$\frac{\partial F(W)}{\partial W} = \begin{pmatrix} 0 & 1 & 0 \\ -u^2 + \chi_{eq} + 1/2\kappa_{eq}u^2 & (2-\kappa_{eq})u & \kappa_{eq} \\ (-H + \chi_{eq} + 1/2\kappa_{eq}u^2)u & H - \kappa_{eq}u^2 & (1+\kappa_{eq})u \end{pmatrix} \tag{2.5}$$

where

$$\chi_{eq} = \left(\frac{\partial p}{\partial \rho}\right)_{\epsilon}, \tag{2.6}$$

$$\kappa_{eq} = \left(\frac{\partial p}{\partial \epsilon}\right)_{\rho}. \tag{2.7}$$

The equilibrium speed of sound is :

$$a_{eq}{}^2 = \chi_{eq} + \kappa_{eq}(H - \frac{1}{2}u^2)$$

To end this paragraph, we notice that, since the partial densities are functions of the total density and the internal energy, we have the following expression for χ_{eq} and κ_{eq} :

$$\chi_{eq} = \sum_{i=1}^{ns} \chi^{fr}{}_i \left(\frac{\partial \rho_i}{\partial \rho}\right)_{\epsilon}, \tag{2.8}$$

$$\kappa_{eq} = \sum_{i=1}^{ns} \chi^{fr}{}_i \left(\frac{\partial \rho_i}{\partial \epsilon}\right)_{\rho} + \kappa_{fr}. \tag{2.9}$$

where $\chi^{fr}{}_i$ and κ_{fr} are :

$$\chi^{fr}{}_i = \frac{\partial p}{\partial \rho_{i\,|\epsilon,\rho_j,j\neq i}}$$

$$\kappa_{fr} = \frac{\partial p}{\partial \epsilon_{\,|\rho_i}}$$

A straightforward calculation gives :

$$\kappa_{fr} = \kappa_{fr} = \kappa \left[1 - \frac{\sum_{i=1}^{ns} Y_i \frac{de^i_{vib}}{dT}}{c_v + \sum_{i=1}^{ns} Y_i \frac{de^i_{vib}}{dT}}\right] = \Phi_1(Y_1, \cdots, Y_{ns}, \frac{de^1_{vib}}{dT}, \cdots, \frac{de^{nv}_{vib}}{dT})$$

$$\chi^{fr}{}_i = c_{v_i}(\kappa_i - \kappa_{fr})T - \kappa_{fr}h_i{}^0 - \kappa_{fr}e_{vib}{}^i = \Phi_2(Y_1, \cdots, Y_{ns}, T, e_{vib}{}^1, \cdots, e_{vib}{}^{nv}, \frac{de^1_{vib}}{dT}, \cdots, \frac{de^{nv}_{vib}}{dT}) \tag{2.10}$$

These expressions will enable us to derive the Roe average in the equilibrium situation.

Chapter 3

A Roe average for equilibrium flows

This section is divided in two parts. In the first one, we recall the expression of the Roe average which have been derived in the case of a mixture of non reacting gases (see [1]) then we show how to use this average to derive a Roe average for chemical equilibrium mixtures.

3.1 A Roe average for non reacting mixtures

The details of the derivation can be found in [1].

We consider a mixture of ns gases. The expression of the internal energy and pressure are the same as in Section 2.1. The set of independents variables which describes the state of the mixture is :

$$W = (\rho_1, \cdots, \rho_{ns}, \rho u, e)$$

Vector W obeys the Euler equations in which the flux $F(W)$ is :

$$F(W) = \Big(\rho_1 u, \cdots, \rho_{ns} u, \rho u^2 + p, u(e+p)\Big)$$

A straightforward calculation shows that the Jacobian matrix A has the following functional form :

$$A = \mathcal{H}\left(u, Y_1, \cdots, Y_{ns}, H, T, {e_{vib}}^1, \cdots, {e_{vib}}^{nv}, \frac{d{e_{vib}}^1}{dT}, \cdots, \frac{d{e_{vib}}^{nv}}{dT}\right)$$

where H is the total enthalpy, Y_i is the mass fraction of species i.

Let us consider two states, W_L and W_R. The Roe averaged matrix between these states is a matrix $\overline{A}(W_L, W_R)$ such that :

- $F(W_L) - F(W_R) = \overline{A}(W_L, W_R).(W_L - W_R)$
- $\overline{A}(W_L, W_R)$ is diagonalizable and has real eigenvalues

A natural condition to impose on $\overline{A}(W_L, W_R)$ is to find back Roe's original results for a single calorically perfect gas. If one admits this and if one assume the following expression of $\overline{A}(W_L, W_R)$:

$$\overline{A}(W_L, W_R) = \mathcal{H}\left(\overline{u}, \overline{Y_1}, \cdots, \overline{Y_{ns}}, \overline{H}, \overline{T}, \overline{e_{vib}{}^1}, \cdots, \overline{e_{vib}{}^{nv}}, \overline{\frac{de_{vib}{}^1}{dT}}, \cdots, \overline{\frac{de_{vib}{}^{nv}}{dT}}\right)$$

then we get ($\mathcal{R}(f)$ is $\dfrac{\sqrt{\rho_L} f_L + \sqrt{\rho_R} f_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}$) :

$$\begin{aligned} \overline{u} &= \mathcal{R}(u) \\ \overline{Y_i} &= \mathcal{R}(Y_i) \\ \overline{H} &= \mathcal{R}(H) \end{aligned}$$

and the additional condition :

$$\Delta p = \sum_{i=1}^{ns} \overline{\chi_i{}^{fr}} \Delta \rho_i + \overline{\kappa^{fr}} \Delta \epsilon \tag{3.1}$$

The latter one can easily be satisfied if one assumes (see equation 2.10) :

$$\begin{aligned} \overline{\kappa^{fr}} &= \Phi_1(\overline{Y_1}, \cdots, \overline{Y_{ns}}, \overline{\frac{de_{vib}^1}{dT}}, \cdots, \overline{\frac{de_{vib}^{nv}}{dT}}) \\ \overline{\chi_i{}^{fr}} &= \Phi_2(\overline{Y_1}, \cdots, \overline{Y_{ns}}, \overline{T}, \overline{e_{vib}{}^1}, \cdots, \overline{e_{vib}{}^{nv}}, \overline{\frac{de_{vib}^1}{dT}}, \cdots, \overline{\frac{de_{vib}^{nv}}{dT}}) \end{aligned} \tag{3.2}$$

with

$$\begin{aligned} \overline{T} &= \mathcal{R}(T) \\ \overline{e_{vib}{}^i} &= \mathcal{R}(e_{vib}{}^i) \end{aligned}$$

and

$$\overline{\frac{de_{vib}{}^i}{dT}} = \begin{cases} \frac{\Delta e_{vib}{}^i}{\Delta T} & \text{if } \Delta T \neq 0 \\ \frac{de_{vib}{}^i}{dT} & \text{else} \end{cases}$$

Moreover, one can show that $\overline{A}(W_L, W_R)$ is diagonalizable and has real eigenvalues (see appendix). These expressions can easily be generalized to mixtures with partial thermal nonequilibrium and the eigenvalues remain real numbers.

3.2 Definition of a Roe average in the equilibrium case

As in the frozen case, since we want to find back Roe's original results for a single perfect gas, the major difficulty for finding a Roe average for the Jacobian matrix of the Euler

equations in the equilibrium case is to find "averaged" values of χ_{eq} and κ_{eq} which satisfy the following relation on the pressure jump Δp , the variation of density $\Delta\rho$ and that of internal energy $\Delta\epsilon$ between two states W_L and W_R :

$$\Delta p = \overline{\chi}\Delta\rho \ + \ \overline{\kappa}\Delta\epsilon$$

The basic remark for building our version of a Roe average for the Jacobian matrix of the Euler equations in the equilibrium case is the following : since

$$\chi_{eq} = \sum_{i=1}^{ns} \chi^{fr}{}_i \left(\frac{\partial \rho_i}{\partial \rho}\right)_\epsilon$$
$$\kappa_{eq} = \sum_{i=1}^{ns} \chi^{fr}{}_i \left(\frac{\partial \rho_i}{\partial \epsilon}\right)_\rho + \kappa_{fr},$$

the idea is to find "averaged" derivative values for the partial densities ρ_i, $\overline{\frac{\partial \rho_i}{\partial \rho}}$ and $\overline{\frac{\partial \rho_i}{\partial \epsilon}}$ and set :

$$\overline{\chi_{eq}} = \sum_{i=1}^{ns} \overline{\chi}^{fr}{}_i \overline{\left(\frac{\partial \rho_i}{\partial \rho}\right)}_\epsilon$$
$$\overline{\kappa_{eq}} = \sum_{i=1}^{ns} \overline{\chi}^{fr}{}_i \overline{\left(\frac{\partial \rho_i}{\partial \epsilon}\right)}_\rho + \overline{\kappa}_{fr}.$$

where $\overline{\chi}^{fr}{}_i$ and $\overline{\kappa}_{fr}$ are given by (3.2).

The only condition to impose on the averaged derivatives of the partial density is to verify :

$$\Delta\rho_i = \overline{\frac{\partial \rho_i}{\partial \rho}} \ \Delta\rho \ + \ \overline{\frac{\partial \rho_i}{\partial \epsilon}} \ \Delta\epsilon \qquad (3.3)$$

This can be easily verified with the help of equation (3.1). In the next paragraph, we will show how to compute averaged derivatives which fulfill (3.3). Unfortunately, there is not uniqueness of thederivation.

3.3 Defining a convenient averaging

In this section, we intend to discuss what average is the best to use . This is not a trivial question since there is no more guide in finding the right answer as the Roe average for perfect gases was a guide in [1] or [14].

To do this, we will rely on a simple principle which is satisfied by the exact derivatives : their expressions do not depend on any linear combinations of the chemical reactions used to define a set of equations verified by the equilibrium mixture. This

condition means that, whatever be the independent algebraic combination of independent equations in system (2.3), we find the same expression of the derivative of partial mass. Moreover, when one changes the set of variables used to write these equations (say mass fractions instead of molar masses), the expressions of the derivatives are only modified by the Jacobian matrix of the change of variables.

The independency of the final solution on any combination of equations in system (2.3)-(2.4) can be formalized in the following way : find two averaging functions "$a \longmapsto \overline{a} = \frac{a_L + Da_R}{1+D}$" and "$a \longmapsto \underline{a} = \frac{Da_L + a_R}{1+D}$" such that for any functions a and b of the state variable W we have :

$$\Delta ab = \overline{a}\ \Delta b\ +\ \overline{b}\ \Delta a = \underline{a}\ \Delta b\ +\ \underline{b}\ \Delta a$$
$$\overline{ab} = \overline{a}\overline{b}$$

Let us recall that, in general, the Δ operator satisfies :

$$\Delta(ab) = \overline{a}\Delta b\ +\ \overline{a}\Delta a \tag{3.4}$$

Unfortunately, these two conditions cannot be true together since the first one is equivalent to :

$$\overline{a} = \frac{a_L + a_R}{2}$$

while the second one is equivalent to :

$$\overline{a} = \sqrt{a_L a_R}.$$

In the sequel, we have chosen to use the arithmetic mean instead of the geometric mean because of the property (3.4).

This implies the choice if the form of the system of equation which define the composition of the mixture. We have chosen the form

$$\begin{array}{ll} [O] = \sqrt{K'_1(T)}\sqrt{[O_2]} & K'_1(T) \equiv \sqrt{K_1(T)} \\ [N] = K'_2(T)\sqrt{[N_2]} & K'_2(T) \equiv \sqrt{K_2(T)} \\ [NO] = K'_3(T)\sqrt{[O_2]}\sqrt{[N_2]} & K'_3(T) \equiv \dfrac{K_3(T)}{\sqrt{K_1(T)}\sqrt{K_2(T)}} \end{array} \tag{3.5}$$

because the equilibrium constants K'_1, K'_2, K'_3 are smooth functions the limits of which, for small temperature, are zero. Moreover, this way of writing the equations (together with (2.4)) leads to the simultaneous solution of two quadratic polynomials in $\sqrt{[O_2]}$ and $\sqrt{[N_2]}$. It is easy to write an iterative algorithm which converges very fastly. Hence, the computation of the "averaged" derivative of the partial densities will be consistent with the algorithm we use to compute the equilibrium states.

Before ending this paragraph, we must write down the expression of $\Delta(abc)$, since products of three terms will be encountered. There are several ways for writing it, but the most symmetric is :

$$\Delta(abc) = \widetilde{ab}\,\Delta c + \widetilde{bc}\,\Delta a + \widetilde{ac}\,\Delta b$$

where

$$\widetilde{ab} = \frac{2\overline{ab} + \overline{a}\,\overline{b}}{3}$$

3.4 Computation of the variation of the partial densities

In fact, we will show how to calculate the variation of the molar mass. The expressions will be given in terms of ΔT and $\Delta\rho$. This is equivalent to what we want because it is possible to express ΔT in terms of $\Delta\rho$ and $\Delta\epsilon$; indeed

$$\Delta\epsilon = \left(\sum_{i=1}^{ns}\left[c_{v_i}\overline{T} + h_i{}^0 + \overline{e_{vib}{}^i}\right]\Delta\rho_i\right) + \left(\sum_{i=1}^{ns}\overline{Y_i}\left[c_{v_i} + \frac{\Delta e_{vib}{}^i}{\Delta T}\right]\right)\Delta T,$$

and because $\Delta\rho_i$ will be given in term of ΔT and $\Delta\epsilon$.

To simplify the writing, let us denote $x \equiv \sqrt{[O_2]}$ and $y \equiv \sqrt{[N_2]}$. The system (2.4)-(3.5) is then equivalent to :

$$\begin{array}{l} x^2 + \left(K'_3\, y + K'_1\right) x - \alpha\rho = 0 \\ y^2 + \left(K'_3\, x + K'_2\right) y - \beta\rho = 0 \end{array} \tag{3.6}$$

The values of α and β are obtained by considering that the sum of partial density is the total one and by using equation (2.4).

If we apply the Δ operator to (3.6), we get :

$$\left\{\begin{array}{l} A\,\Delta x + B\Delta y = \alpha\,\Delta\rho + \mathcal{A}\Delta T \\ A'\,\Delta x + B'\Delta y = \beta\,\Delta\rho + \mathcal{B}\Delta T \end{array}\right. \tag{3.7}$$

where

$$\left\{\begin{array}{l} A = 4\overline{x} + \widetilde{K'_3}\,y + \overline{K}'_1 \\ B = \widetilde{K'_3}\,x \\ A' = \widetilde{K'_3}\,y \\ B' = 4\overline{y} + \widetilde{K'_3}\,x + \overline{K}'_2 \\ \mathcal{A}\Delta T = -\widetilde{xy}\,\Delta K'_3 - \overline{x}\Delta K'_1 \\ \mathcal{B}\Delta T = -\widetilde{xy}\,\Delta K'_3 - \overline{y}\Delta K'_2 \end{array}\right. \tag{3.8}$$

It is always possible to solve the linear system (3.7-3.8) : the determinant remains positive. Then, it is trivial that Δx and Δy have a linear dependency in the variables $(\Delta T, \Delta \rho)$.

Now, from (3.5), we have :

$$\begin{aligned}
\Delta[O_2] &= 2\overline{x}\Delta x \\
\Delta[N_2] &= 2\overline{y}\Delta y \\
\Delta[O] &= \overline{K'_1}\,\Delta x + \overline{x}\Delta K'_1 \\
\Delta[N] &= \overline{K'_2}\,\Delta y + \overline{y}\Delta K'_2 \\
\Delta[NO] &= x\widetilde{K'_3}\,\Delta y + y\widetilde{K'_3}\,\Delta x + \overline{xy}\Delta K'_3
\end{aligned} \tag{3.9}$$

This ends the proof.

Remark : If $\Delta T = 0$, the expressions $\Delta K'_i$ are replaced by the derivatives of K'_i.

Chapter 4

Test cases

To validate the solver we propose, we consider 3 test cases. The first and the second one are 1D shock tubes which have been proposed by Montagne [6]. The third one is a difficult test case which have been proposed in the Hypersonic Workshop held in January 1990 at Antibes (France).

The numerical scheme relies on a finite-volume approach. The 1D test cases are computed by a second-order MUSCL predictor-corrector scheme where slope limitation is applied on the characteristic variables. The 2D test case have been solved by a first order explicit scheme.

4.1 1 D test cases

They are defined as follows :

		Density kg/m^3	Pressure N/m^2	Temp. K	Energy $(m/sec)^2$	Velocity m/sec	Mach
Case A	left	.066	$9.84\ 10^4$	4390	$7.22\ 10^6$	0	0
	right	0.03	$1.50\ 10^4$	1378	$1.44\ 10^6$	0	0
Case B	left	1.	$6.50\ 10^5$	2242	$2.00\ 10^6$	0	0
	right	.010	$1.\ 10^3$	346	$2.50\ 10^5$	0.	0.

Case A is a shock tube with a moderate density and energy ratio. The resulting shock wave is of moderate strength but significant real gas effects are found in this temperature range. Case B is a shock tube with very large density and energy ratios, it produces a large transsonic expansion wave. In each cases, the initial distribution of mass fraction was obtained assuming chemical equilibrium [5].

For each case, we present the density, velocity, Mach number, pressure. In all cases, a regular mesh of 100 points was used.

Discussion As it can be seen, no particular problems have been encountered. The results are given on Figures A.1. for case A and Figure A.2 for case B. The solutions compare very well with Montagne's. In particular, the expansion waves are accurately simulated. The slight oscillations which can be seen on the pressure and the velocity in Figure A.1 may have two origins. First, the jump in temperature is very important so very important real gas effects are involved. The second possible origin in inherent to the discretization : it is easy to show that in the case of two non reacting gases, even in a supersonic contact discontinuity, the pressure cannot remain constant because the ratio of specific heat (κ in Section 2.1) which is given by the numerical algorithm is not correct (see [13] for more details). This is also true for any upwind scheme, even if Godunov's Riemann solver is used.

4.2 2D Test case

Now, we use the first-order scheme, on a structured mesh, to solve the flow around a simple ellipse with angle of attack of 30 degrees and a Mach number of 25. The pressure at infinity is $p = 2.54Pa$ and the temperature is $T = 205.3K$. This test case have been proposed as number 6.3-4 in the 1990 Hypersonic Workshop.

The mesh has 91 $\times$ 31 points. On the surface of the ellipse, the numerical flux is given by applying Roe's solver to two states with opposite normal velocity and the same tangential velocity. The other boundary conditions are classical. The initial condition corresponds to an impulsive start. The maximum CFL number is set to 0.4. We use Harten's entropy correction in order to obtain the correct physical solution.

Discussion We were not able to run the code directly with the initial conditions as stated above because on the upper part of the body, the pressure tended to become extremely low if not negative. So we started with the same flow at zero degre of incidence during 100 iterations and then turned to the true outflow conditions.

With such a procedure, no particular problem was encountered and convergence was very smooth (see Figure A.4).

We have plotted in Figure A.3 the temperature and O_2 lines and the values of the Mach number and $C_p = \frac{p_\infty - p}{1/2\rho_\infty u_\infty^2}$ on the body surface.

The chemical transition zone can clearly be seen on the temperature lines below the upper part of the shock wave. This zone corresponds to the dissociation of oxygen.

On the plot of C_p, the low pressure on the upper part of the ellipse can clearly be seen.

Chapter 5

Conclusion

In this report, we have developed a new version of Roe's Riemann solver adapted to chemically equilibrium flows. It is based upon an extension of the same Riemann solver adapted to mixtures of frozen flows and it applies to class of algebraic chemistry models.

We have not yet been able to prove that the Roe averaged Jacobian matrix has real eigenvalues ; nevertheless, in appendix, we have shown that the "frozen" solver has this property. Since the chemistry model is very smooth, we conjecture that for convex equation of state, the averaged Jacobian matrix has this property in practice.

This new solver has been tested on several 1D test cases and on a difficult 2D one. The regularity of the solutions and the smoothness of the convergence in the 2D case show its efficiency.

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Appendix A

About the eigenvalues of $\overline{A}(W_L, W_R)$

In this section, we want to show that the eigenvalues of $\overline{A(W_L, W_R)}$ are real, which reduces to show that $\overline{a}^2$ is positive.

Let us recal that

$$\overline{a}^2 = \sum_{i=1}^{ns} \overline{\chi_i}\overline{Y_i} \; + \; \overline{\kappa}_{fr} \left(\overline{H} - \frac{1}{2}\overline{u}^2 \right)$$

If we make the convention that for $i \leq nv + 1$, ${e_{vib}}^i = 0$, we have :

$$\overline{\chi_i} = c_{v_i}(\kappa_i - \overline{\kappa}_{fr})\overline{T} - \overline{\kappa}_{fr} \left({h_i}^0 + \overline{{e_{vib}}^i} \right),$$

$$\overline{\kappa}_{fr} = \frac{\sum_{i=1}^{ns} \overline{Y}_i R_i}{\sum_{i=1}^{ns} \overline{Y}_i c_{v_i} + \frac{\Delta {e_{vib}}^i}{\Delta T}}$$

It has been noticed by several authors that

$$\overline{H} - \frac{1}{2}\overline{u}^2 = \overline{h} + \frac{\rho}{2(\sqrt{\rho_L} + \sqrt{\rho_R})^2}(\Delta u)^2$$

with

$$\overline{h} = \sum_{i=1}^{ns} \left(c_{v_i}(1 + \kappa_i)\overline{Y_i T} + \overline{Y}_i {h_i}^0 + \overline{{e_{vib}}^i Y_i} \right)$$

If ${e_{vib}}^i$ is a monotone increasing function as in the case of interest here, $\overline{\kappa}_{fr} \geq 0$, the problem reduces to show that

$$\tilde{b}^2 = \sum_{i=1}^{ns} \overline{\chi_i}\overline{Y_i} \; + \; \overline{\kappa}_{fr}\overline{h} \geq 0.$$

Some algebra gives

$$\begin{aligned}\frac{\tilde{b}^2}{\kappa_{fr}} &= \overline{T}\sum_{i=1}^{nv}\overline{Y}_i\frac{\Delta e_{vib}{}^i}{\Delta T} + \sum_{i=1}^{ns} c_{v_i}\gamma_i\overline{Y_iT} + \sum_{i=1}^{nv}\left(\overline{Y_ie_{vib}{}^i} - \overline{Y_ie_{vib}{}^i}\right) \\ &\leq \overline{T}\sum_{i=1}^{nv}\overline{Y}_i\frac{\Delta e_{vib}{}^i}{\Delta T} + \sum_{i=1}^{nv}\left(\overline{Y_ie_{vib}{}^i} - \overline{Y_ie_{vib}{}^i}\right) \ .\end{aligned} \tag{A.1}$$

Now, let us notice that for any function $\mathcal{D}$ of W :

$$\overline{Y_i\mathcal{D}} - \overline{Y}_i\overline{\mathcal{D}} = \frac{\sqrt{\rho_L\rho_R}}{\left(\sqrt{\rho_L}+\sqrt{\rho_R}\right)^2}\ \Delta Y_i\Delta\mathcal{D}\ .$$

The right hand side of equation (A.1) becomes :

$$\sum_{i=1}^{nv}\frac{\Delta e_{vib}{}^i}{\Delta T}\left(\overline{TY}_i - \frac{\sqrt{\rho_L\rho_R}}{\left(\sqrt{\rho_L}+\sqrt{\rho_R}\right)^2}\Delta Y_i\Delta T\right) \tag{A.2}$$

Let us examine the terms between brackets. Since

$$\overline{Y}_i = Y_{iL} + \frac{\sqrt{\rho_R}}{\sqrt{\rho_L}+\sqrt{\rho_R}}\Delta Y_i$$

and

$$\overline{T} = T_R - \frac{\sqrt{\rho_L}}{\sqrt{\rho_L}+\sqrt{\rho_R}}\Delta T,$$

we deduce that each term between brackets satisfy :

$$\overline{TY}_i - \frac{\sqrt{\rho_L\rho_R}}{\left(\sqrt{\rho_L}+\sqrt{\rho_R}\right)^2}\Delta Y_i\Delta T = T_LY_{iL} + \frac{\sqrt{\rho_L}}{\sqrt{\rho_L}+\sqrt{\rho_R}}\Delta(T\ Y_i) \tag{A.3}$$

By definition,

$$\Delta(T\ Y_i) = T_RY_{iR} - T_LY_{iL} \geq -T_LY_{iL}$$

thus the term in equation (A.3) is greater than

$$\frac{\sqrt{\rho_L}}{\sqrt{\rho_L}+\sqrt{\rho_R}}T_LY_{iL} \geq 0 \tag{A.4}$$

For the case of interest, we have already noticed that $\frac{\Delta e_{vib}{}^i}{\Delta T} \geq 0$, so the results of equations (A.1), (A.2), (A.3), (A.4) indicate that the square of the averaged speed of sound is positive.

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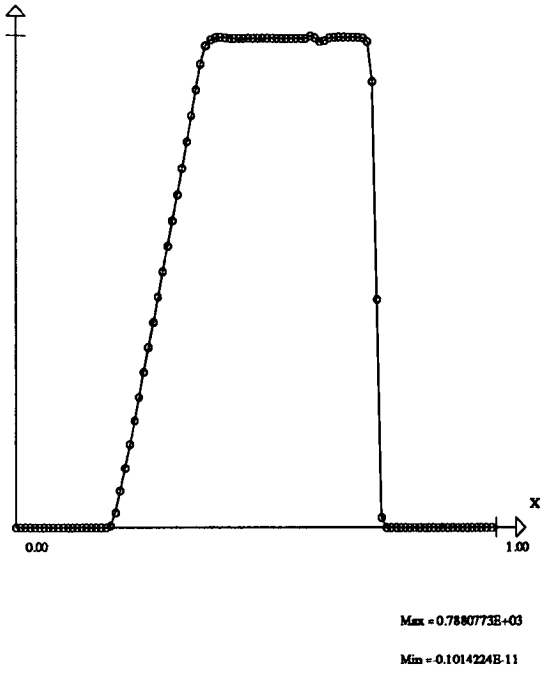
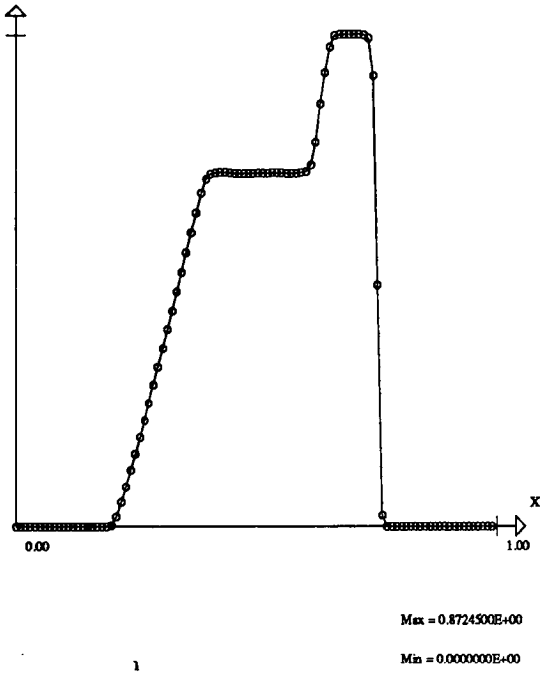
Figure A.1: Case A



Velocity



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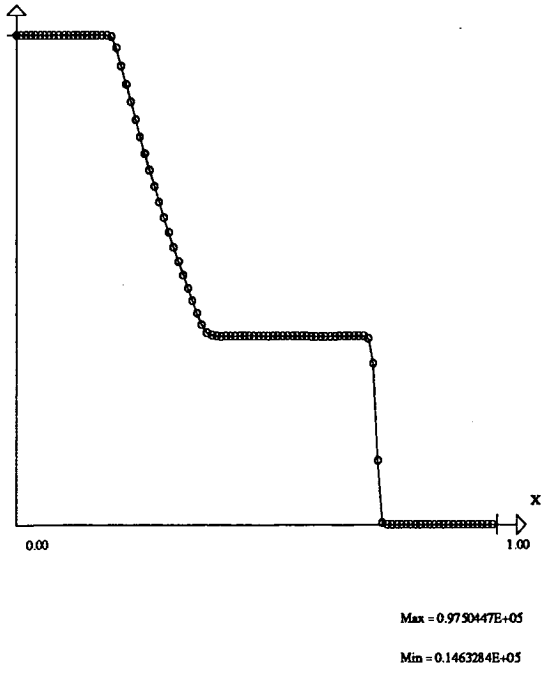
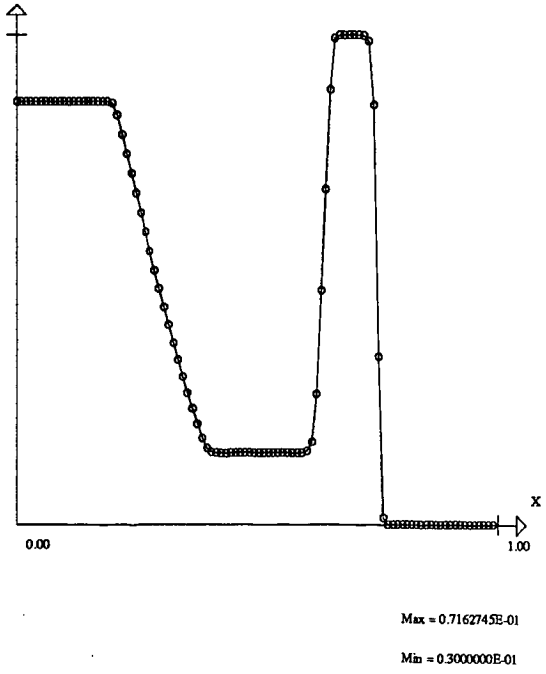
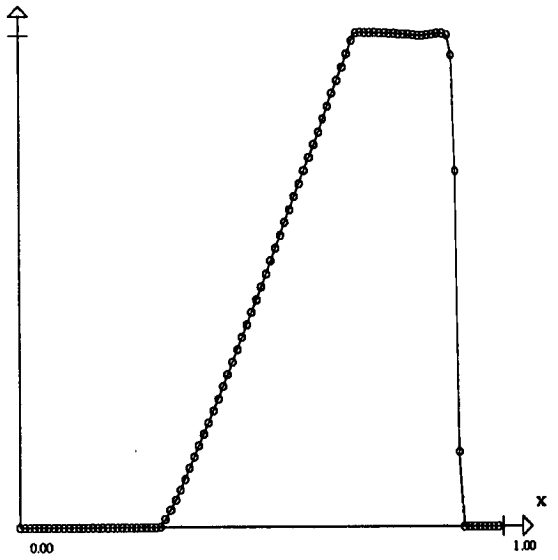


Pressure

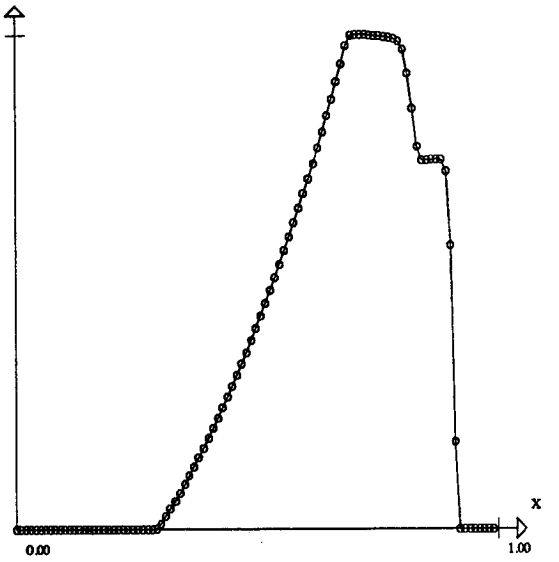


Density

Figure A.2: Case B



Velocity



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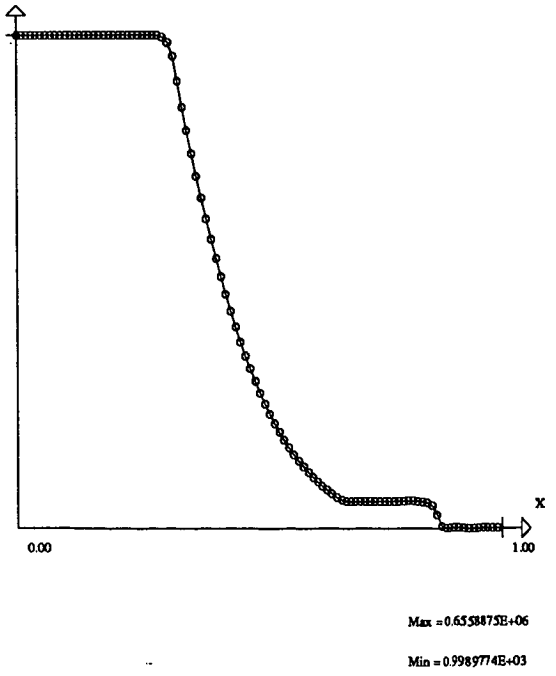
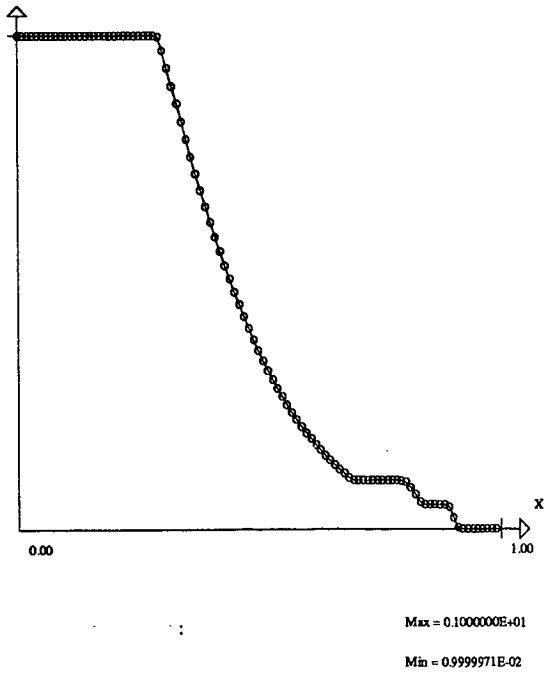


Pressure



Density

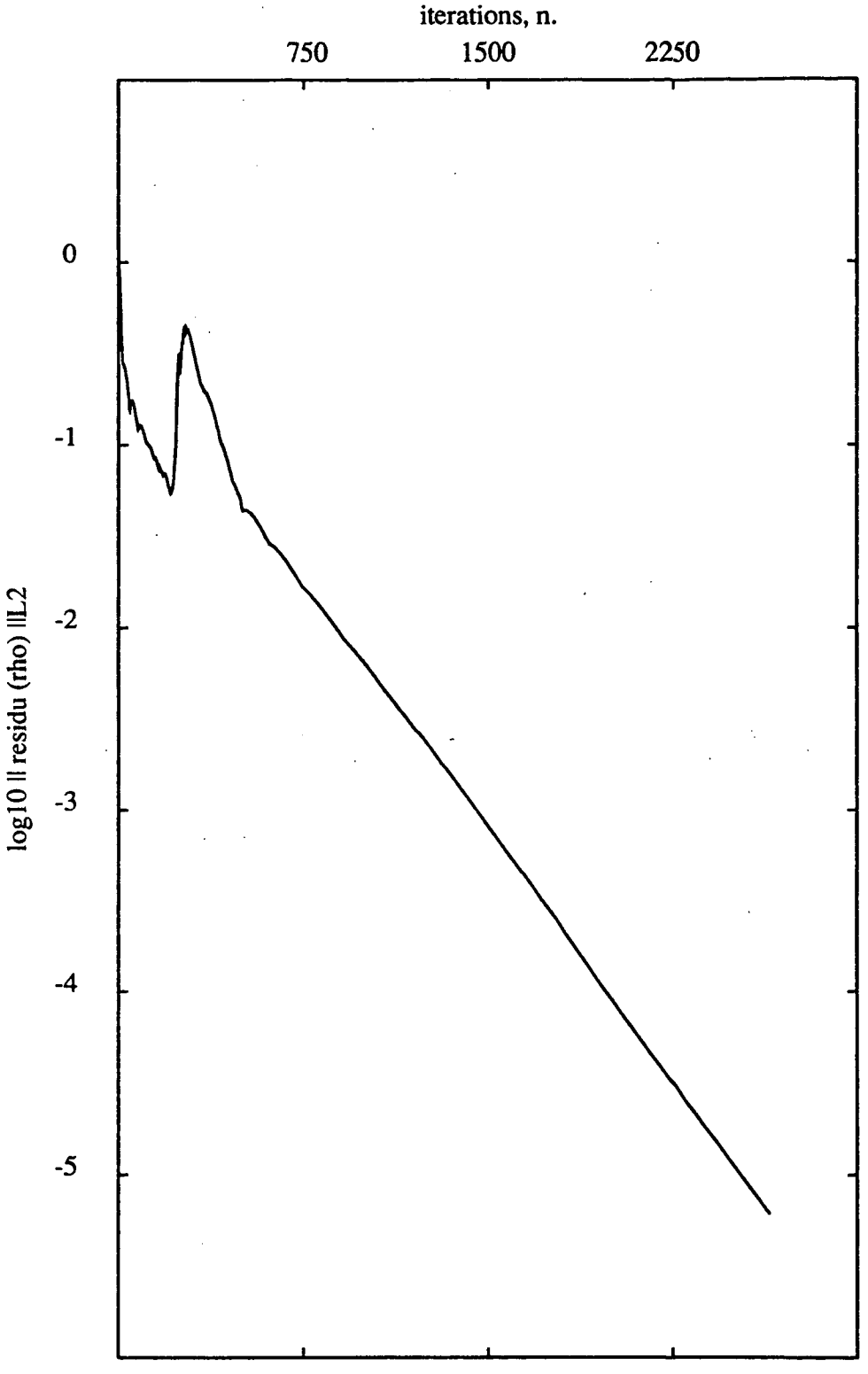
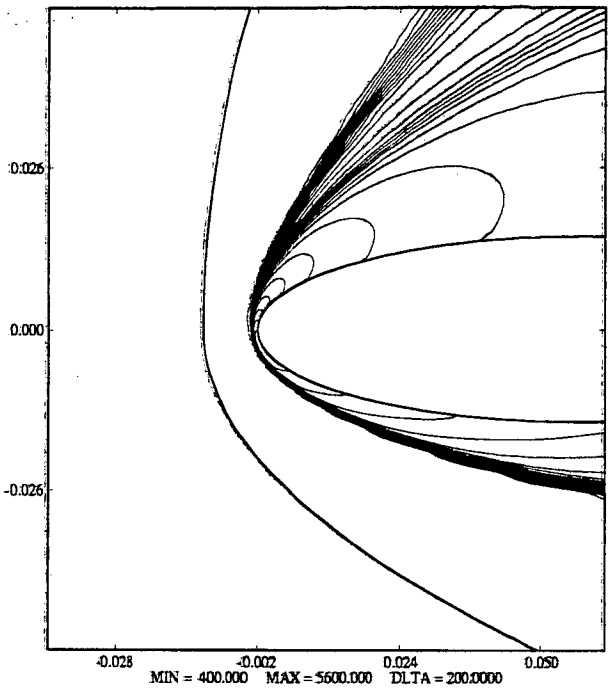

- MACH=25.000 - INCIDENCE=30.000 -
iterations, n.
750
1500
2250
0
-1
-2
-3
-4
-5
log10 || residu (rho) ||L2

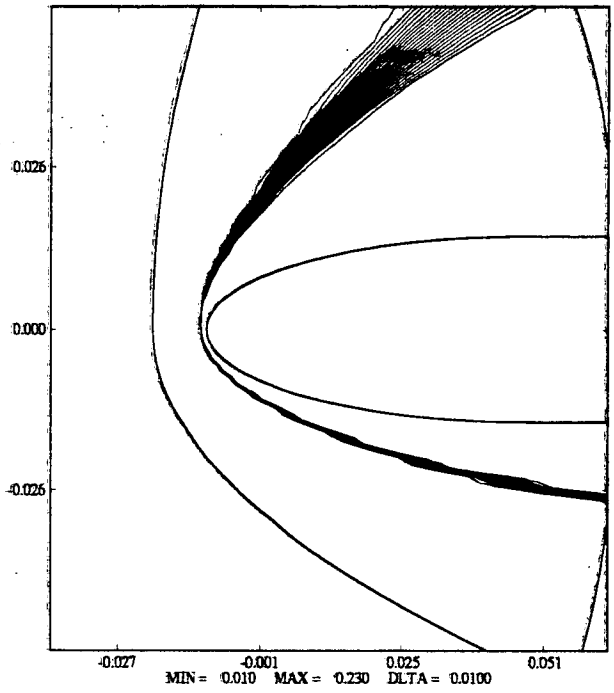
Figure A.4

Figure A.3: Simple ellipse at $M_\infty = 25$ and 30° incidence



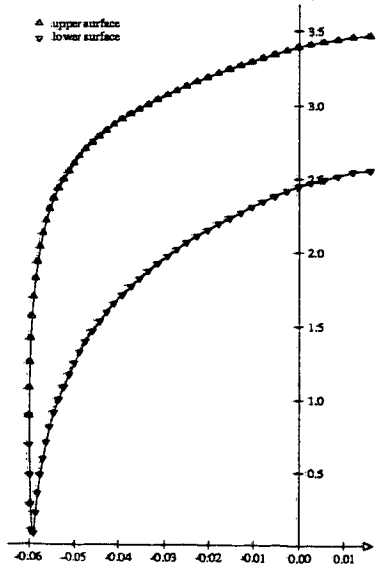
Temperature

Min = 203.2 K, Max = 5768 K, $\Delta T = 200$ K



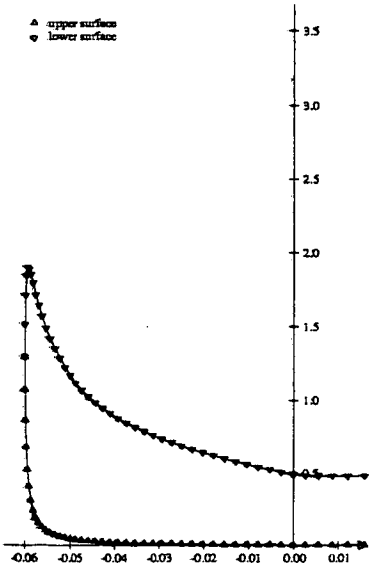
Y_{O_2} lines

Min = 0., Max = 0.233, $\Delta Y = 0.01$



Mach number

Min = 0.07, Max = 3.466



C_p on the body

Min = −1.898, Max = −0.002

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